Quantum Phase Transitions with Cold Polar Molecules

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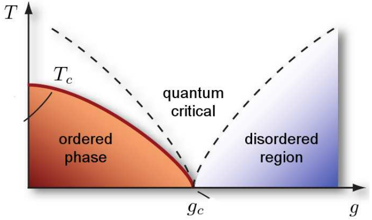
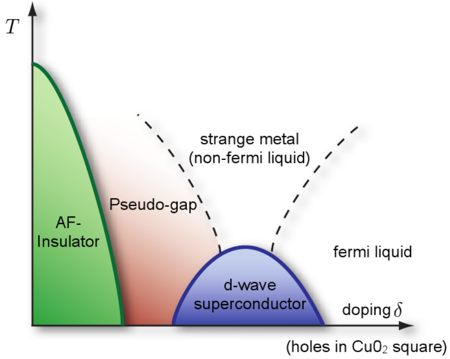
Outline

Quantum Phase Transitions

Quantum phase transitions ...

- are driven by quantum fluctuations
- identified by non–analytical points in the ground state energy
- accessible by varying a physical parameter g at $T = 0$



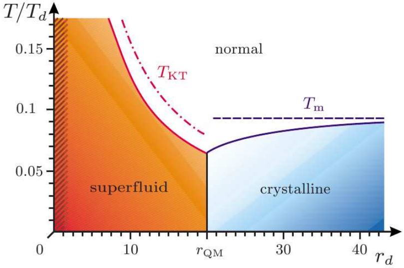


Interesting quantum phase transition are

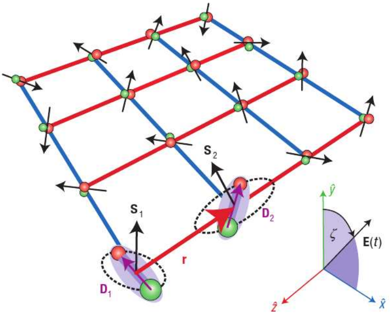
- order $\longleftrightarrow$ disorder
- supersolid $\longleftrightarrow$ superfluid
- High–T_C superconductors

Mimicking Condensed Matter Systems

- Realizations of spin models
- Search for "exotic" phases that do not fit into Landau theory
  - Topological phases
  - Critical spin liquids
- Heisenberg antiferromagnet on triangular (or Kagomé) lattice



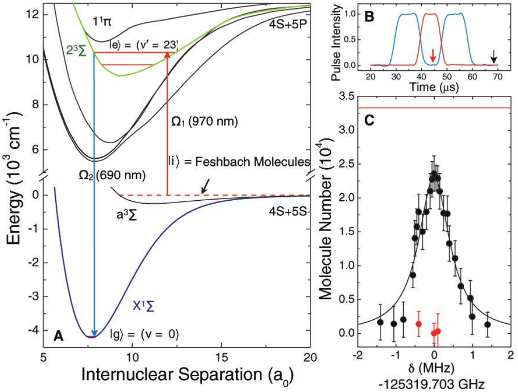
[A.Micheli, PRL–A76, 043604(2007)]



[A.Micheli, Nat-Phys–287(2006)]

- Cold polar molecules in optical lattices offer possibilities to
  - realize and control strongly correlated quantum states
  - simulate spin models in the strong coupling limit

Experiments with Cold Polar Molecules

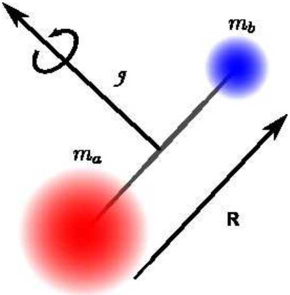


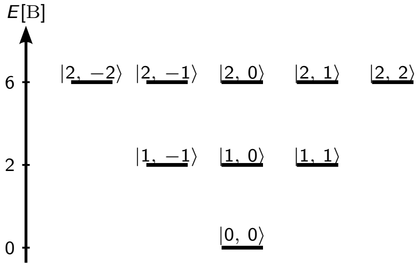
[Jun Ye et al, Science Vol. 322(2008)]

- Experimental realization with photo–association
- Polar molecules are prepared in their rotational & vibrational ground state

Properties of Polar Molecules

- Hetero–nuclear molecules (partial charges)
- electronic–, roto-vibrational– and rotational excitations
- Polar molecules are sensitive to external electric fields in dipole approximation
  - permanent dipole moments $\approx 1 \ldots 10\,\mathrm{debye}$





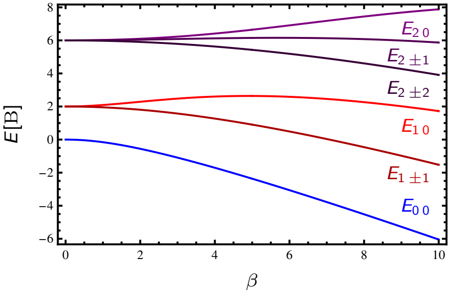
- Only rotor excitations $\approx 1 \ldots 100\,\mathrm{GHz}$ ("microwaves")
  - Cold molecules near electronical–, vibrational– and rotational ground state
  - Rigid rotor $\mathcal{H} = B\mathcal{J}^2$

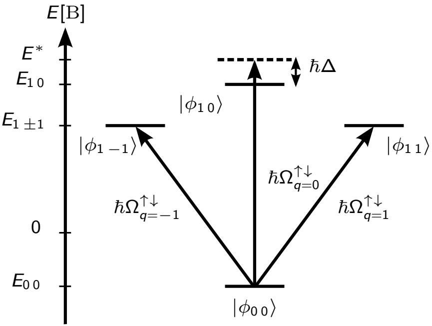
Polar Molecules in External Fields

- Rigid rotor in static electric fields

$$\mathcal{H} = B\mathcal{J}^2 - d_0 E_{\mathrm{dc}}$$

  - leads to a dc–Stark shift





- Coupling to microwave fields E_{ac} with polarization q and frequency ω_L

$$\mathcal{H} = B\mathcal{J}^2 - d_0 E_{\mathrm{dc}} - \mathbf{d} \cdot \mathbf{E}_{\mathrm{ac}}(t)$$

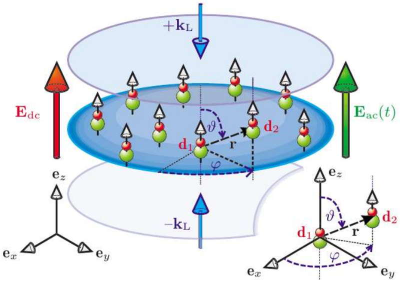
  - leads to an ac–Stark shift with excitation gap $\Delta E = \hbar\sqrt{\Delta^2 + \Omega_0^2}$ and detuning $\Delta = \omega_L - \omega$

Interacting Polar Molecules in Optical Traps

- The optical trap can be realized by a pair of circularly polarized counter propagating laser beams

$$\mathbf{E}_{\text{opt}}(\mathbf{r}) = E_{\text{opt}} \cos\left(\frac{\omega_L}{c} z\right) \mathbf{e}_1$$

trapping the molecules in the xy–plane



[A.Micheli, PRL–A76, 043604(2007)]

- The Hamiltonian describing a single molecule

$$\mathcal{H}(t) = \frac{\mathbf{p}^2}{2m} + \mathcal{V}_{\text{trap}} + B\mathcal{J}^2 - d_0 E_{0\text{dc}} - \mathbf{d} \cdot \mathbf{E}_{\text{ac}}(t)$$

- Strong dipole–dipole interactions are tunable with external fields

$$\mathcal{V}_{\text{dd}} = \frac{\mathbf{d}_1 \cdot \mathbf{d}_2 - 3(\mathbf{d}_1 \cdot \mathbf{e}_r)(\mathbf{e}_r \cdot \mathbf{d}_2)}{r^3}$$

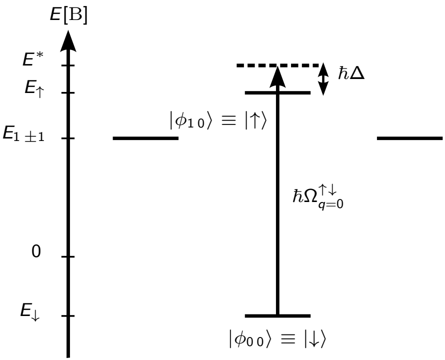
Realizing the *XXZ* Model

- The Hamiltonian in the RWA reads

$$\mathcal{H} = -\frac{\hbar}{2}\begin{pmatrix} \Delta & \Omega_0 \\ \Omega_0 & -\Delta \end{pmatrix} + E_{0,0}\mathbb{1}$$

- RWA accounts for energy conservation

$e^{i\omega_L t} \approx 0$ emission of a photon	$e^{i(\omega_L+\omega)t} \approx 0$ emission and activation
$e^{-i\omega_L t} \approx 0$ absorption and deactivation	$e^{-i(\omega_L+\omega)t} \approx 0$ absorption of a photon



- Coupling of $|\phi_{0\,0}\rangle$ and $|\phi_{1\,0}\rangle$ with linear polarized microwaves
- Near resonant coupling to satisfy dipole approximation and rotating wave approximation
- Induced dipole moments

  $d_0^{\uparrow\uparrow} = \langle\uparrow| d_0 |\uparrow\rangle$, $d_0^{\downarrow\downarrow} = \langle\downarrow| d_0 |\downarrow\rangle$

  and $d_0^{\uparrow\downarrow} = \langle\uparrow| d_0 |\downarrow\rangle$

Realizing the *XXZ* Model

- Spin–1/2 XXZ model for many body systems on a square lattice

$$\mathcal{H} = J \underbrace{\sum_{i,j=1}^{N} \left(\sin\vartheta \frac{\mathcal{S}_{ix}\mathcal{S}_{jx} + \mathcal{S}_{iy}\mathcal{S}_{jy}}{\left|\mathbf{R}_i - \mathbf{R}_j\right|^3} + \cos\vartheta \frac{\mathcal{S}_{iz}\mathcal{S}_{jz}}{\left|\mathbf{R}_i - \mathbf{R}_j\right|^3} \right)}_{\text{Dipol–Dipole Interaction}} - \underbrace{\sum_{i=1}^{N} \mathbf{h}_i \cdot \mathbf{S}_i}_{\text{single molecules}}$$

with separation vector $\mathbf{r}_i = a\mathbf{R}_i$, "spin" $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$, and "magnetic" field $\mathbf{h}$

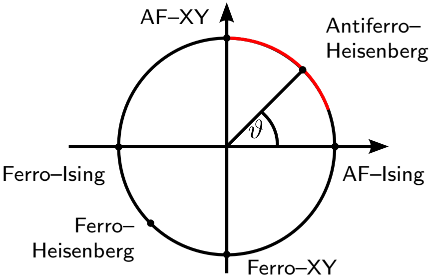
- Different coupling strength: In–axis J_z and in–plane $J_\perp$

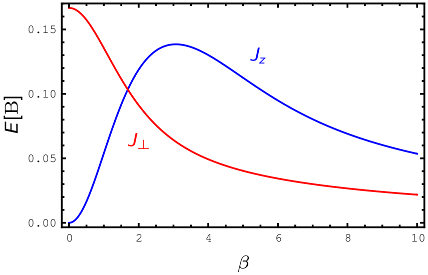
$$J_\perp = J\sin\vartheta = \frac{2\left(d_0^{\uparrow\downarrow}\right)^2}{\hbar^2 a^3} \qquad J_z = J\cos\vartheta = \frac{\left(d_0^{\uparrow\uparrow} - d_0^{\downarrow\downarrow}\right)^2}{\hbar^2 a^3}$$

$$\mathbf{h} = -N\Omega_0\mathbf{e}_x + N\left(-\Delta + \frac{\left(d_0^{\uparrow\uparrow}\right)^2 - \left(d_0^{\downarrow\downarrow}\right)^2}{2\hbar a^3}\sum_{j=1}^{N}\frac{1}{R_j^3}\right)\mathbf{e}_z$$

Tuning of Coupling Constants

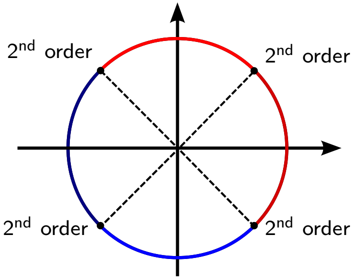
- The detuning Δ can be chosen such that $h_z = 0$
- $h_x = \Omega_0$ needed for relaxation, small due to weak coupling
- By varying $\beta = {}^{dE_{\mathrm{dc}}}/_{B} \longrightarrow$ different models depending on the angle $\vartheta(\beta)$



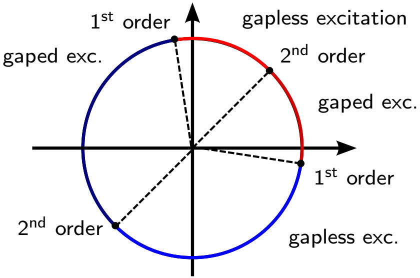


- For $J_\perp = J_z \Rightarrow \vartheta = {}^{\pi}/_{2}$
  - Heisenberg antiferromagnet realizable for $\beta \approx 1.6876$
  - minimal possible $\vartheta \approx 90^\circ \ldots 19.7^\circ$

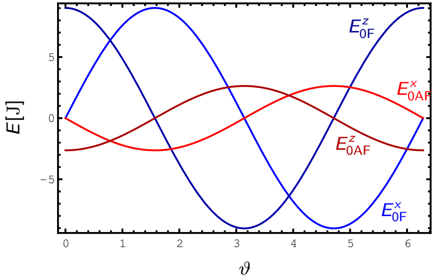
Phase Diagram of the XXZ Model



Nearest neighbor interaction



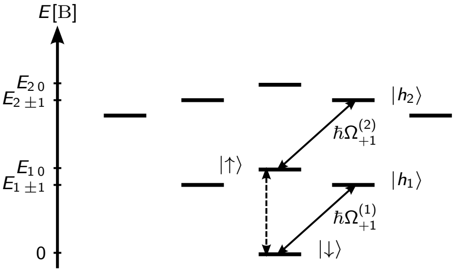
$^1/_{r^3}$–interaction



- Applying a spin wave analysis about mean field ground state
- Influence of the dipolar interaction shifts critical point

Realization of the $t - J$ Model

- Allow hopping of molecules in lattice
- Doping with holes by leaving vacancies
- Explore strong coupling limit $t/U \ll 1$
- Three parameters to adjust $\mathbf{h} = 0$, $J_z = J_\perp = J$ and $-J/4$



- t-J Model describing strongly correlated electronic systems

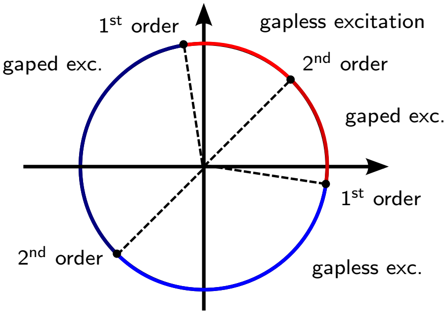
$$\mathcal{H} = -t \sum_{\langle i,j\rangle\sigma}^{N} \left(c^\dagger_{i\sigma} c_{j\sigma} + c_{i\sigma} c^\dagger_{j\sigma} \right) + J \sum_{i,j=1} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right)$$

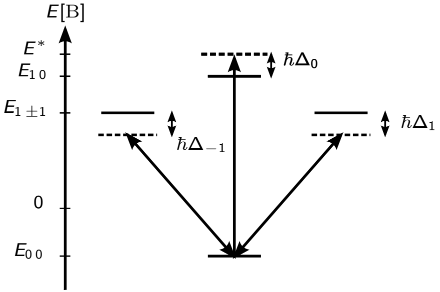
with $J = 4t^2/U$ and U being the Coulomb repulsion

Summary and Outlook

Polar Molecules in optical lattices are convenient as ...

- Quantum simulator for antiferromagnets
- Spin models with frustration (e.g. no Neél ordering)





- Additional coupling to the ground state to realize $t - J$ model exactly
- Realization of ferro–electrics via coupling all four states